FYS3150 – Project 4

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Abstract

In this project we study the Ising model of ferromagnetism in 2D, with no external magnetic field. In particular, we are looking at the system as a model for a phase transition. We employ the Metropolis algorithm, and attempt to extract a behaviour of the model at different temperatures, lattice sizes, and times (number of Monte Carlo cycles). We find that increasing the lattice size drastically increases the required computation time, meaning we are constrained to smaller lattice sizes for this project. However, even for the small lattices we used in this project, we could see indications of a phase transition.

We used the data gathered with small lattice sizes in order to extrapolate to the case of $L = \infty$, and find a reasonable approximation to the critical temperature.

1 Physical background

A magnet is a material that produces a magnetic field, and responds to external magnetic fields. A magnet consiting of many microscopic dipoles that only responds to external magnetic field is called a paramagnet. However, the dipole-dipole interaction in the material will generally make the dipoles favour an antiparalell state. That is, all else beeing equal, the individual dipoles will tend to align in the opposite direction of its neighbours, making the perfect paramagnet an idealiced case.

A material in which the individual dipoles tend to align themselves paralell to their neighbours is called ferromagnetic. In Iron, for example, there are quantum mechanical exchange forces that give this anti-intuitive effect.

In a ferromagnet we can get a spontaneous magnetization even without an external magnetic field. However this only occurs at temperatures below a critical temperature called the Curie temperature, T_c, after Pierre Curie. Above this temperature a ferromagnet essentially becomes a paramagnet.

2 The Ising model

In the Ising model we assume that the dipoles, (we will call them spins), can be in only two possible states. That is, they can only be either "up" or "down", $s = \pm 1$. We further assume that all the spins are in a uniform grid formation. We also assume that the interaction is only between the nearest neighbours. The energy of interaction between two neighbouring spins is then: $e = -J$, if the spins are paralell and $e = J$ if they are anti-paralell (J is just a constant of interaction, with units of energy).

The total enery of a system is then given by the sum of all the energies of interaction, plus the sum of the energy given by the interaction of each spin with the external magnetic field. In this project we have no external magnetic field. The total energy is then given by the sum:

$$E = -J \sum_{<i,j>} s_i s_j,$$

where $< i, j >$ in the sum denotes a sum over nearest neighbours only.

2.1 Modeling liquid-vapour phase transition

We can use the Ising model for systems other than a ferromagnet. If instead of thinking of each point like a spin, we consider each point like a point in space that can either be occupied or not occupied by a molecule of a gas (we call it the lattice gas). Spin up corresponds to a state being occupied, and spin down corresponds to not being occupied. The model assumes that there is a small energy of interaction that favours two adjacent states being occupied. The magnetization is then replaced by the density, and the chemical potential represents the external magnetic field.

The spontaneous transition between the two magnetization states then corresponds to a phase transition in the lattice gas, liquid $\rightarrow$ vapour e.g.

We must note that the symmetry between the two states of magnetization in the ferromagnet do not transfer over to the gas model. This is because there is no interaction between two empty points in the lattice. This means that while the phase transition in the ferromagnet model occurs when the external field is zero, $H = 0$. In the lattice gas model, the phase transition occurs when the chemical potential has a non-zero (negative) value, $\mu \neq 0$.

2.2 Mean field approximation

To solve the Ising model is in general very hard, but we can make a useful approximation called the mean field approximation. If we look at a single spin at a random point in the system, s_i. The energy of interaction with its neighbours is then:

$$E_i = -J \sum_{<j>} s_i s_j = -Jns_i\bar{s},$$

where $\bar{s}$ is the average spin of the neighbours, and n is the number of neighbours.

We can now calculate the partition function for this individual spin:

$$Z_i = e^{\beta Jn\bar{s}} + e^{-\beta Jn\bar{s}} = 2\cosh(\beta Jn\bar{s}).$$

We can then find the expectation value of our spin, $\bar{s}_i$:

$$\bar{s}_i = m = \frac{1}{Z_i}\left[e^{\beta Jn\bar{s}} - e^{\beta Jn\bar{s}}\right] = \tanh(\beta Jn\bar{s}). \tag{1}$$

If each spin has many neighbours, we can make the further assumption: The average spin of the neighbours of each individual spin, is equal to the average spin over the entire system:

$$m = \bar{s}. \tag{2}$$

We can then find the different values for m that fulfills both these criteria by plotting the two equations, (1) and (2), in the same figure (see figure 1).

In the case where we get three solutions, the two nontrivial solutions corresponds to spontaneous magnetization of the magnet and are stable, while the trivial solution $m = 0$ corresponds to a unstable solution.

We see that the number of solutions are dependent on the value of β, the critical case is when $Jn\beta = 1$. If β has a lower bound in order to produce spontaneous magnetization, that means that there is a upper bound on the temperature in order to produce spontaneous magnetization, this critical temperature is the Curie temperature, $T_c = nJ/k$.

For 2 dimensions, the number of neighbours is $n = 4$, so $kT_c/J = 4$. In the exact solution this number should be $kT_c/J \approx 2.269$, so the mean field approximation is pretty bad in two dimensions. This is obvious if we think about the assumption we made about the neighbours, they were supposed to have the same average magnetization as the global average. This is a very good approximation if we have alot of neighbours, but understanably a bad one when we only have four.

Although the mean field approximation gives inaccurate results, we can still use it to understand what is going on in our model. We can, for example, plot the mean spontaneous magnetization versus temperature (see figure 2). We can here clearly see the phsyical meaning of the Curie temperature.

3 Closed form solution, 2 x 2 lattice

In the case of $L = 2$, using periodic boundary conditions, where L is the number of spins in each dimension, we can find closed form expressions for the quantaties $\langle E \rangle$, $\langle |\mathcal{M}| \rangle$, C_V, and χ.

$E = -8J$	$\mathcal{M} = \pm 4$	$\begin{bmatrix}\uparrow & \uparrow \\ \uparrow & \uparrow\end{bmatrix}$ $\begin{bmatrix}\downarrow & \downarrow \\ \downarrow & \downarrow\end{bmatrix}$
$E = 0$	$\mathcal{M} = +2$	$\begin{bmatrix}\downarrow & \uparrow \\ \uparrow & \uparrow\end{bmatrix}$ $\begin{bmatrix}\uparrow & \downarrow \\ \uparrow & \uparrow\end{bmatrix}$ $\begin{bmatrix}\uparrow & \uparrow \\ \downarrow & \uparrow\end{bmatrix}$ $\begin{bmatrix}\uparrow & \uparrow \\ \uparrow & \downarrow\end{bmatrix}$
	$\mathcal{M} = -2$	$\begin{bmatrix}\uparrow & \downarrow \\ \downarrow & \downarrow\end{bmatrix}$ $\begin{bmatrix}\downarrow & \uparrow \\ \downarrow & \downarrow\end{bmatrix}$ $\begin{bmatrix}\downarrow & \downarrow \\ \uparrow & \downarrow\end{bmatrix}$ $\begin{bmatrix}\downarrow & \downarrow \\ \downarrow & \uparrow\end{bmatrix}$
	$\mathcal{M} = 0$	$\begin{bmatrix}\uparrow & \uparrow \\ \downarrow & \downarrow\end{bmatrix}$ $\begin{bmatrix}\downarrow & \downarrow \\ \uparrow & \uparrow\end{bmatrix}$ $\begin{bmatrix}\uparrow & \downarrow \\ \uparrow & \downarrow\end{bmatrix}$ $\begin{bmatrix}\downarrow & \uparrow \\ \downarrow & \uparrow\end{bmatrix}$
$E = 8J$	$\mathcal{M} = 0$	$\begin{bmatrix}\uparrow & \downarrow \\ \downarrow & \uparrow\end{bmatrix}$ $\begin{bmatrix}\downarrow & \uparrow \\ \uparrow & \downarrow\end{bmatrix}$

Figure 3: Possible configurations of the 2×2-system. $\uparrow$ and $\downarrow$ denote spin up, and spin down, respectively. Energies and magnetization, E and $\mathcal{M}$, given for each state.

The possible states of the 2×2-lattice case is shown in figure 3, with corresponding energies and magnetizations. In order to find closed form expectation values for E and $\mathcal{M}$, aswell as for the specific heat, C_V, and the succeptibility, χ, we first need to find an expression for the partition function, Z. It is defined as the sum of the Boltzmann factor, $\exp(-\beta E_i)$, over all possible microstates of the system.For our specific case, this yields

$$\begin{aligned} Z &= \sum_{i=1}^{M} e^{-\beta E_i} = 12e^{-0\beta J} + 2e^{8\beta J} + 2e^{-8\beta J} \\ &= 12 + 2\left(e^{-8\beta J} + e^{8\beta J}\right) \\ &= 4\left[\cosh\left(8\beta J\right) + 3\right]. \end{aligned} \tag{3}$$

We have that the expectation value of the energy, $\langle E \rangle$, is given as

$$\langle E \rangle = \frac{1}{Z} \sum_{i=1}^{M} E_i e^{-\beta E_i} = -\frac{1}{Z} \frac{\partial}{\partial \beta} Z \,,$$

where we used that

$$\begin{aligned} \frac{\partial}{\partial \beta} Z &= \frac{\partial}{\partial \beta} \sum_{i=1}^{M} e^{-\beta E_i} \\ &= \sum_{i=1}^{M} -E_i e^{-\beta E_i} \Rightarrow -\frac{1}{Z} \frac{\partial}{\partial \beta} Z = \langle E \rangle \,. \end{aligned}$$

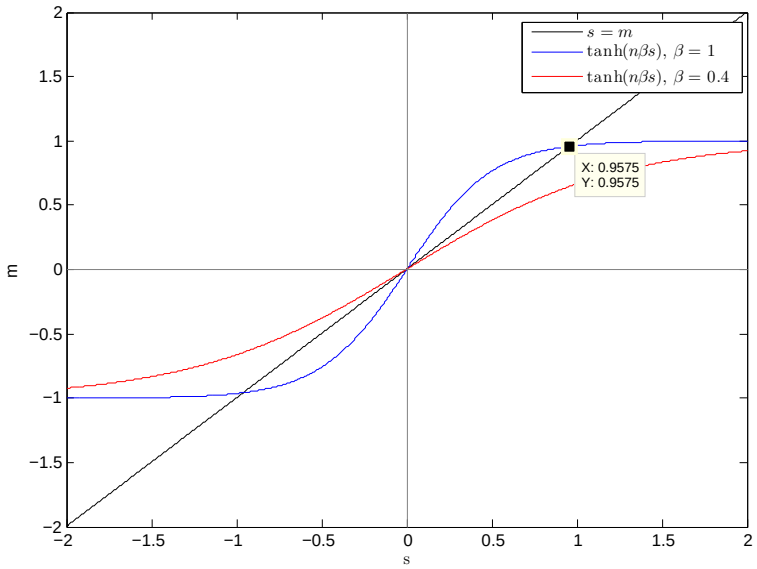

Figure 1: We have set $n = 2$ and $J = 1$. We see that the trivial case $m = 0$ is always a solution, and that if β is higher than a certain value, we get two different solutions.

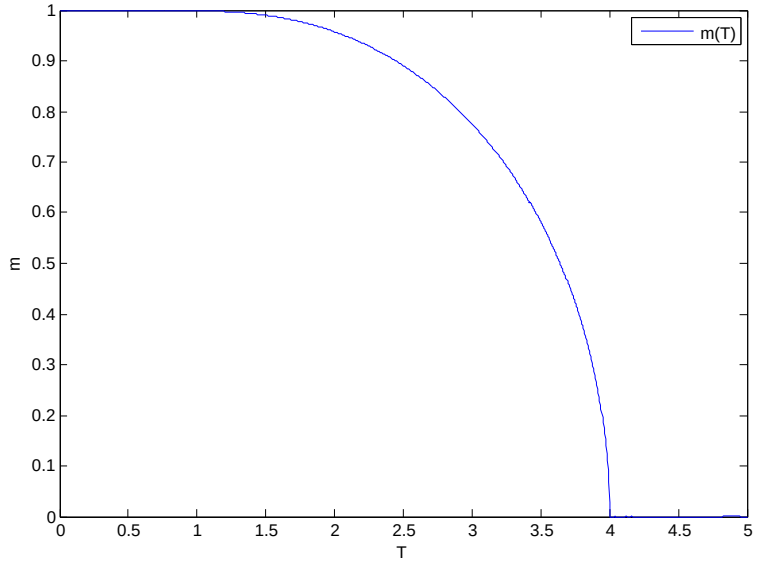

Figure 2: $n = 2$, $J = 1$, we also use the absolute value of the magnetization. We here clearly see the critical temperature of the system. Notice also that the magnetization approaches one very fast when we get below the critical temperature.

Computing now this expectation value gives

$$\begin{aligned}\langle E\rangle &= -\frac{1}{Z}\frac{\partial}{\partial\beta}Z \\ &= -\frac{1}{4\left[\cosh\left(8\beta J\right)+3\right]}\left[32J\sinh\left(8J\beta\right)\right] \\ &= -8J\frac{\sinh(8J\beta)}{\cosh(8J\beta)+3}\,. \end{aligned} \tag{4}$$

Similarily, for the magnetization, we obtain the relation

$$\begin{aligned}\langle|\mathcal{M}|\rangle &= \frac{1}{Z}\sum_{i=1}^{M}|M_i|e^{-\beta E_i} \\ &= -\frac{1}{4\left[\cosh\left(8\beta J\right)+3\right]}\left[2\cdot 4e^{8\beta J}+8\cdot 2e^{0\beta J}\right] \\ &= \frac{8e^{8\beta J}+16}{4[\cosh\left(8\beta J\right)+3]} = \frac{2e^{8\beta J}+4}{\cosh\left(8\beta J\right)+3}\,. \end{aligned} \tag{5}$$

In order to find the specific heat, C_V, we first find the expectation value of E^2, and the expectation value of E, squared.

$$\begin{aligned}\langle E^2\rangle &= \frac{1}{Z}\sum_{i=1}^{M}E_i^2e^{-\beta E_i} \\ &= \frac{1}{4\left[\cosh\left(8\beta J\right)+3\right]}\left[2(-8)^2Je^{8\beta J}+2\cdot 8^2Je^{-8\beta J}\right] \\ &= \frac{32J\left[e^{8\beta J}+e^{-8\beta J}\right]}{\cosh\left(8\beta J\right)+3} = 64J\frac{\cosh(8\beta J)}{\cosh\left(8\beta J\right)+3} \end{aligned} \tag{6}$$

$$\begin{aligned}\langle E\rangle^2 &= \left(\sum_{i=1}^{M}-E_ie^{-\beta E_i}\right)^2 = \left(-8J\frac{\sinh(8J\beta)}{\cosh(8J\beta)+3}\right)^2 \\ &= 64J\frac{\sinh^2(8J\beta)}{\left(\cosh(8J\beta)+3\right)^2} \\ &= 64J\frac{\sinh^2(8J\beta)}{\cosh^2(8J\beta)+6\cosh(8J\beta)+9}\,. \end{aligned} \tag{7}$$

This gives C_V as

$$\begin{aligned}C_V &= \frac{1}{kT^2}\left[\langle E^2\rangle-\langle E\rangle^2\right] \\ &= \frac{64J}{kT^2}\left[\frac{\cosh(8\beta J)}{\cosh\left(8\beta J\right)+3}-\frac{\sinh^2(8J\beta)}{\cosh^2(8J\beta)+6\cosh(8J\beta)+9}\right] \\ &= \frac{64J}{kT^2}\left[\frac{\cosh(8\beta J)}{\cosh\left(8\beta J\right)+3}-\frac{\sinh^2(8J\beta)}{\cosh^2(8J\beta)+6\cosh(8J\beta)+9}\right] \\ &= \frac{64J}{kT^2}\left[\frac{3\cosh(8\beta J)+1}{(\cosh(8\beta J)+3)^2}\right]\,. \end{aligned} \tag{8}$$

We find now the succeptibility, χ, given as $\chi = 1/kT\,(\langle|M|^2\rangle - \langle|M|\rangle^2)$.

$$\begin{aligned}\langle|M|^2\rangle &= \frac{1}{Z}\sum_{i=1}^{M}|M_i|^2 e^{-\beta E_i} \\ &= \frac{1}{4\left[\cosh(8\beta J)+3\right]}\left[2\cdot 4^2 e^{8\beta J} + 8\cdot 2^2 e^{0\beta J}\right] \\ &= \frac{1}{4\left[\cosh(8\beta J)+3\right]}32\left[e^{8\beta J}+1\right] = \frac{8e^{8\beta J}+8}{\cosh(8\beta J)+3}\,. \end{aligned} \tag{9}$$

$$\begin{aligned}\langle|M|\rangle^2 &= \left(\frac{1}{Z}\sum_{i=1}^{M}|M_i|e^{-\beta E_i}\right)^2 = \left(\frac{2e^{8\beta J}+4}{\cosh(8\beta J)+3}\right)^2 \\ &= \frac{4e^{16\beta J}+8e^{8\beta J}+16}{\cosh^2(8J\beta)+6\cosh(8J\beta)+9}\,. \end{aligned} \tag{10}$$

This gives the succeptibility

$$\begin{aligned}\chi &= \frac{1}{kT}\left(\langle|M^2|\rangle - \langle|M|\rangle^2\right) \\ &= \frac{1}{kT}\left[\frac{8e^{8\beta J}+8}{\cosh(8\beta J)+3} - \frac{4e^{16\beta J}+8e^{8\beta J}+16}{\cosh^2(8J\beta)+6\cosh(8J\beta)+9}\right] \\ &= \frac{1}{kT}\frac{4(3+e^{-8\beta J}+5e^{8\beta J})}{(\cosh(8\beta J)+3)^2} \end{aligned} \tag{11}$$

4 Solution algorithm

In order to simulate the behaviour of our system over time, we employ the Metropolis algorithm. As shown earlier, we can derive the partition function, Z, for the $L = 2$ case. For this special case, there are $2^4 = 16$ possible states of the system. However, for an $n \times n$-system, we have 2^{n^2} possible states, which makes the partition function extremely time consuming to compute for $L \geq 2$. This is the major advantage to the Metropolis algorithm — we do not need to find this Z.

The algorithm works by first setting up an intial state of the system, s_0. A random move to another state, $s_0 \rightarrow s_i$, is then proposed. If the new move results in a state of lower energy than s_0, the new move is automatically accepted. If not, the new move is accepted with a given probability. The process is repeated until equilibrium is reached, at which point we can start computing our expectation values.

The algorithm we implemented is here outlined in pseudo-code.

```
set_Initial_State()

while !(equilibrium reached)
   do Monte Carlo cycle

for i=0...n
   do Monte Carlo cycle

   sum up relevant values

expectationVals = expectationVals / n
```

Monte Carlo cycles here denote the propositions of random moves to new states, i.e. flipping spins in our model. A single Monte Carlo cycle is defined as L^2 propositions, which may or may not be

accepted. The reason for defining a single cycle in such a way, is to reduce the correlation between subsequent states. If we call state s_i the state after i cycles, s_i and s_{i+1} would be *very* similar (or equal) if we propose only a single flip per cycle.

The Monte Carlo cycles themselves can be represented in pseudo-code as shown here.

```
for k=0...L^2
   i,j = uniform random in [1,L]

   // compute energy difference for this new proposed state
   dE = newEnergy - oldEnergy

   if (dE <= 0)
      flip spin, accept new configuration
   else if (uniform random in [0,1] < exp(-dE/T))
      flip spin, accept new configuration
   else
      retain old configuration
```

One of the *major* advantages of using the Metropolis algorithm with the Ising model is that the exponential term used to determine if a spin flip is accepted, $e^{-\beta\Delta E}$, has only 5 possible values (in 2D). This means that instead of doing the expensive calculation of this exponential L^2 times for every single Monte Carlo cycle, we can instead compute the possible values it takes beforehand.

In order to implement periodic boundary conditions in our model, we attempted two different approaches. The first was to simply append 2 rows and 2 columns to the matrix representing our spins, and updating the values on the edges every time a spin is flipped on one of the edges. The second approach was to use a $L \times L$-matrix, but instead of indexing into this array using the normal method, `A[i][j+1]`, we instead use the expression `A[i][(i+1+n)%n]`. We found that for smaller lattice sizes, the first method was faster, however for lattices of size $L \gtrsim 25$, the second method performed better.

4.1 Parallelization

Parallelization of the algorithm was fairly straight forward. A single core was used for the first part of the program, in which we allow the system time to equilibrate. After this, we run simultaneous Monte Carlo cycles on four cores, and find four values for the expectation values. These four values are then averaged to produce the final result.

5 Results

5.1 Numerical approximation to the case of 2 x 2 lattice

In order to test the implementation of our algorithm, we compare the computed numerical approximations in the 2×2-case with the previously derived closed form expressions. The results of this test are shown in table 1. Relative errors in the approximations are shown in table 2. Satisfied that our program reproduces the results from the closed form computation, we proceed to the case of $n \times n$-lattice.

We found, somewhat surprisingly, that increasing the number of Monte Carlo cycles performed over $N \gtrsim 10^7$ resulted in increased error. We believe this is because for large values of N we are repeatedly adding a very small value, `E`, to an increasingly large number, `Etot`, which makes us lose precision. This error should be relatively easy to fix, but we did not notice until we were almost finished with the report, and thus did not have time to correct it.

N	time usage, [s]	$\langle E \rangle$	$\langle \lvert M \rvert \rangle$	C_V	χ
10^6	0.4	-7.9845	3.99479	0.123792	0.0157528
10^7	2.4	-7.9839	3.99463	0.128577	0.0160818
10^8	24.0	-7.98404	3.99468	0.127404	0.0159288
∞	—	-7.98393	3.99464	0.128329	0.016043

Table 1: Comparison of closed form, and numerical approximations, for the case of the 2×2-lattice. Time usage shown is for a parallelized version of the code, running on 4 cores. $T = 1$. $N = \infty$ here denotes the closed form expressions derived earlier.

N	time usage, [s]	$\frac{\langle E' \rangle - \langle E \rangle}{\langle E \rangle}$	$\frac{\langle \lvert M \rvert' \rangle - \langle \lvert M \rvert \rangle}{\langle \lvert M \rvert \rangle}$	$\frac{C_V' - C_V}{C_V}$	$\frac{\chi' - \chi}{\chi}$
10^6	0.4	$7.10999 \cdot 10^{-5}$	$3.58152 \cdot 10^{-5}$	0.0353598	0.0180854
10^7	2.4	$3.92586 \cdot 10^{-6}$	$2.93668 \cdot 10^{-6}$	0.00193382	0.00241962
10^8	24.0	$1.45663 \cdot 10^{-5}$	$9.63516 \cdot 10^{-5}$	0.00721317	0.00711623

Table 2: Relative errors in the numerical approximation, for the case of the 2×2-lattice. Time usage shown is for a parallelized version of the code, running on 4 cores. $T = 1$. $\langle E' \rangle$, $\langle M' \rangle$, etc, denote the numerical approximations, while unprimed values represent the exact values.

5.2 How many cycles before a steady state is reached

If we start in the ground state, we are basically in the equilibrium state, atleast for $T = 1$. And for $T = 2.4$ the system varies so much in the equilibrium state that almost every starting position will soon become indistinguishable from a the equilibrium. See figures 4 and 5.

If we start in a random state then typically the net magnetization will be zero, and we are far from the equilibrium for $T = 0$, nevertheless we see that within a couple of hundred Monte Carlo cycles (MC-cycles), we are in the equilibrium. See figures 6 and 7.

5.3 How many cycles needed for a good approximation of $\langle E \rangle$ and $\langle \lvert M \rvert \rangle$

We also want to check how many MC-cycles we need to get a good estimate for $\langle E \rangle$ and $\langle E \rangle$. We see that if we use 10^4 MC-cycles we have a decent approximation. These results are shown in figures 8, 9, 10, and 11.

5.4 The probability of the system being in a state with energy E

When finding the probability distribution $P(E)$ for the two temperatures, 1.0 and 2.4 (in units of kT/J). We simply used the values for the energy we have written to file, and used the histogram function in matlab to display how often each energy was found. Normalizing this histogram gave us, $P(E)$, see figures 12 and 13.

The smallest energy-change possible in the entire system is 4 (in units of J), this corresponds to flipping a spin with three of the four adjacent spins pointing in the same direction, and the fourth pointing in the oposite direction. However the energy 4 units from the ground state is not possible, this is because, in the ground state, all spins will have four neighbours in the same direction. If a spin flips, it will produce an change in energy of 8 units.

5.5 Number of accepted configurations

We run simulations for the lattice size $L = 20$, over temperatures $T \in [0.1, 5.0]$, and plot the probability of accepting configurations as a function of temperature. This is shown in figure 14.

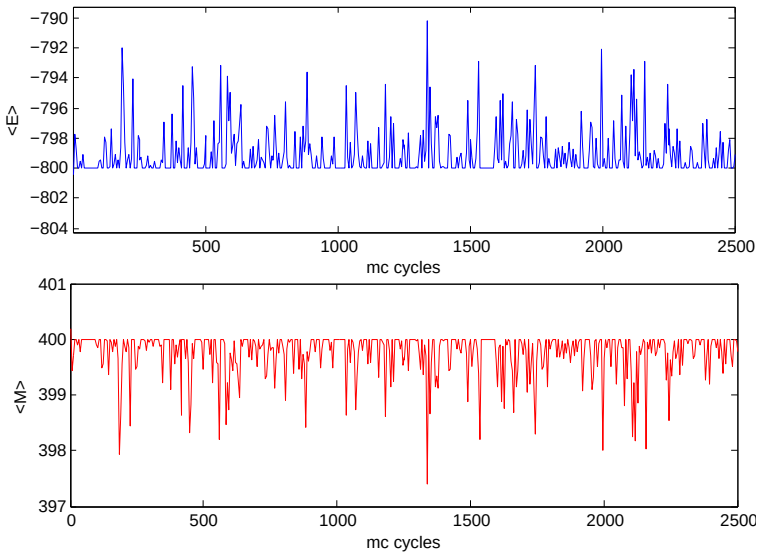

Figure 4: $T = 1.0$, starting in the ground state.

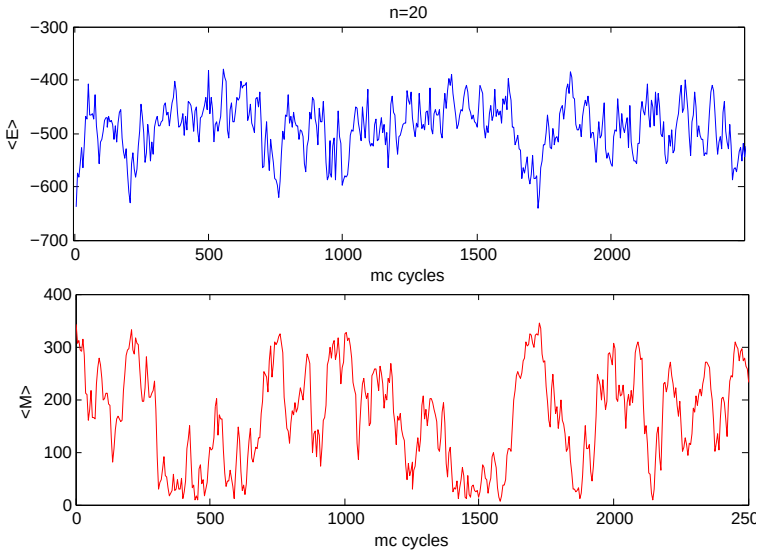

Figure 5: $T = 2.4$, starting in the ground state.

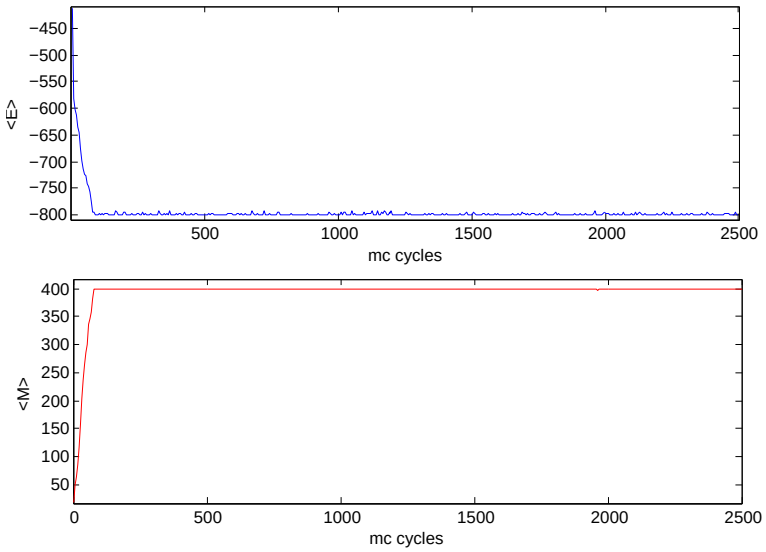

Figure 6: $T = 1.0$, starting in the a random state.

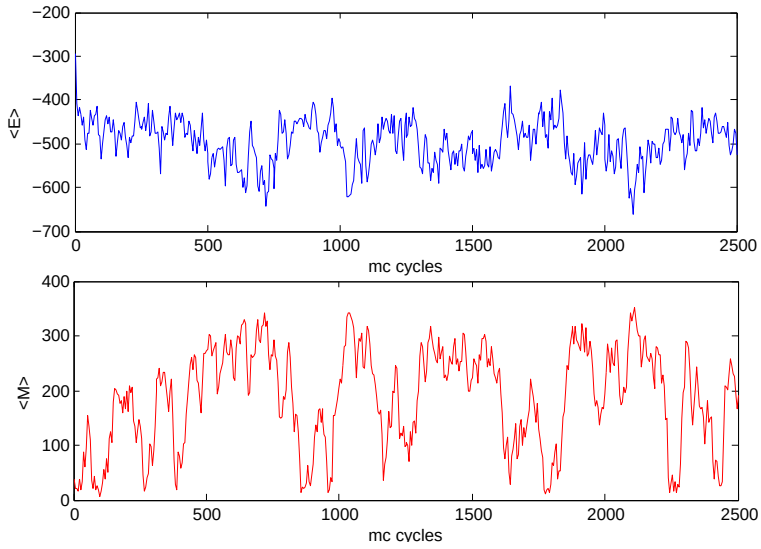

Figure 7: $T = 2.4$, starting in the a random state.

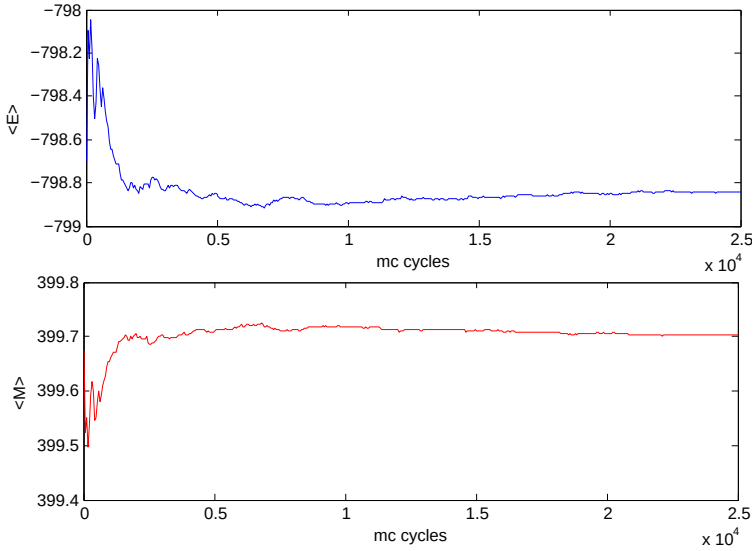

Figure 8: $\langle E \rangle$ and $\langle |M| \rangle$ as functions of the number of Monte Carlo cycles used. $T = 1$, starting in the ground state.

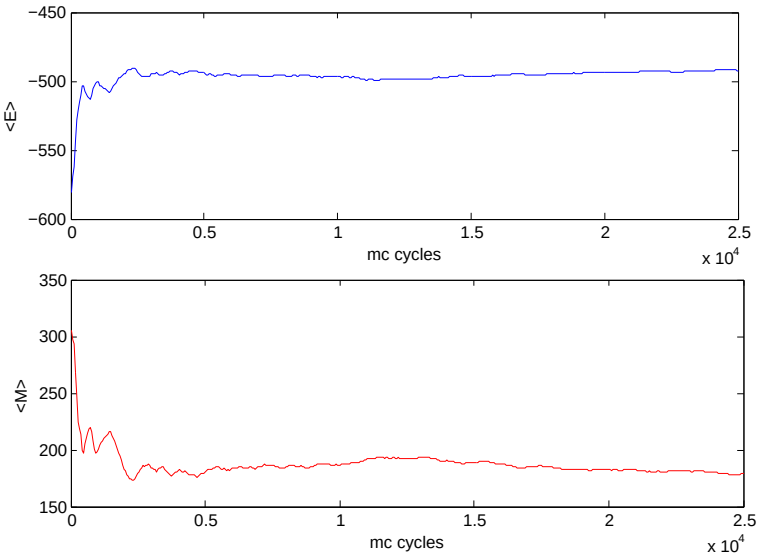

Figure 9: $\langle E \rangle$ and $\langle |M| \rangle$ as functions of the number of Monte Carlo cycles used. $T = 2.4$, starting in the ground state.

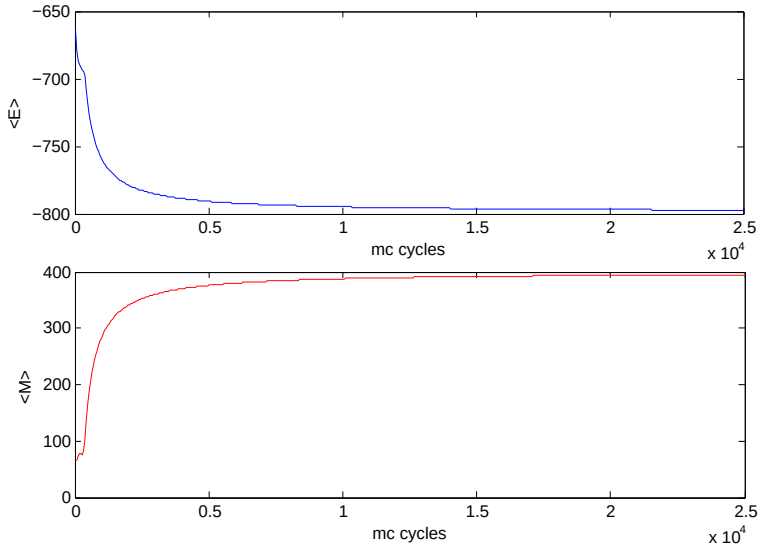

Figure 10: $\langle E \rangle$ and $\langle |M| \rangle$ as functions of the number of Monte Carlo cycles used. $T = 1$, starting in a random state.

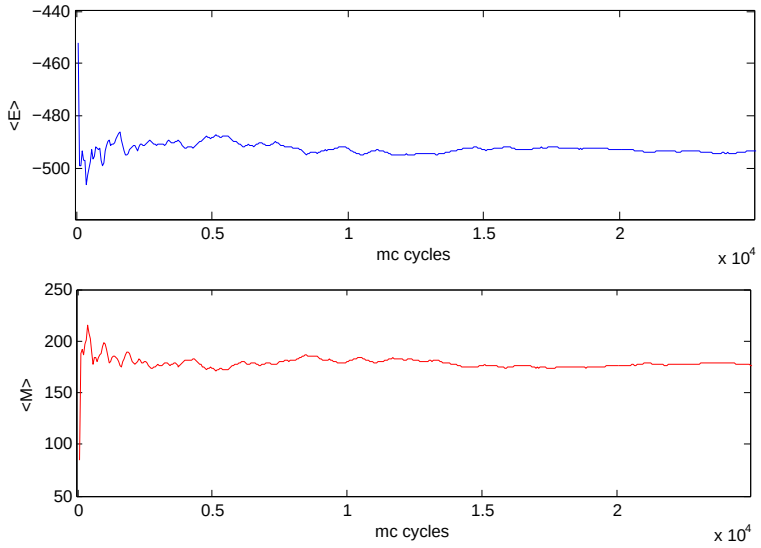

Figure 11: $\langle E \rangle$ and $\langle |M| \rangle$ as functions of the number of Monte Carlo cycles used. $T = 2.4$, starting in a random state.

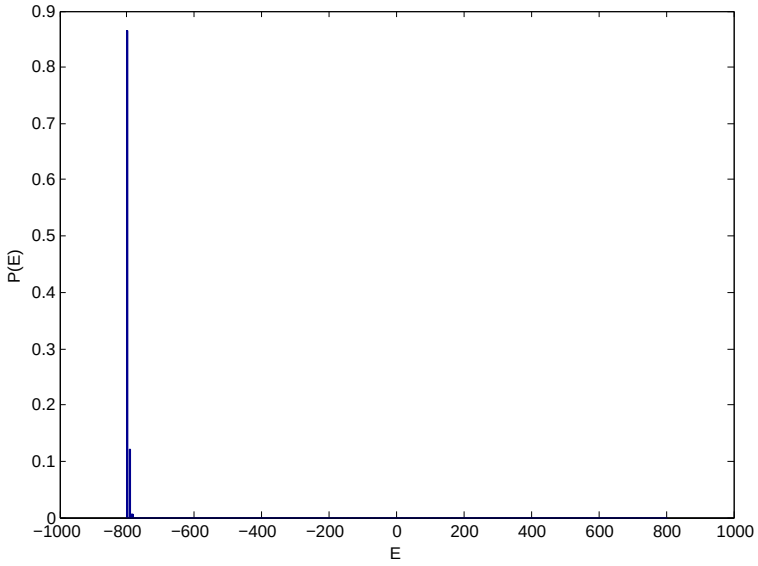

Figure 12: The probability of $P(E)$ of being in a state corresponding to the given energy E. $T = 1$. Numerically approximated $\sigma_E^2 = 9.412$, we see that the variance is of the same order as the jump in energy from the ground state to the first excited state.

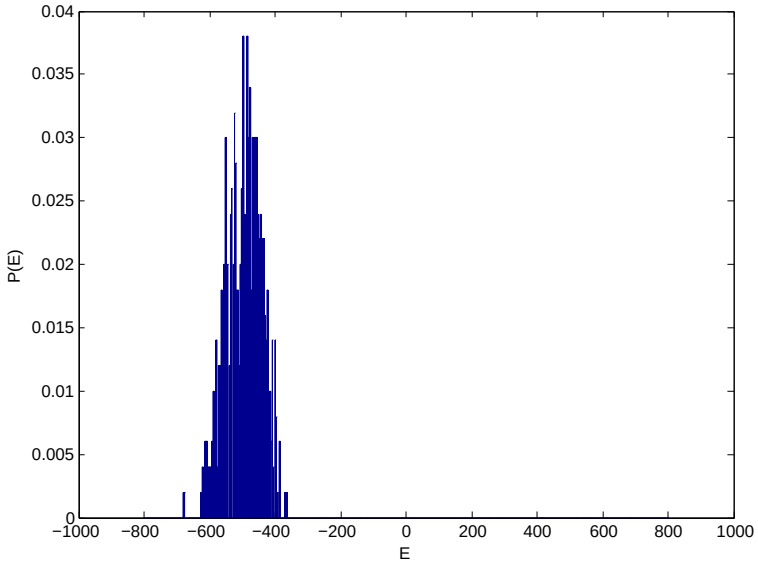

Figure 13: The probability of $P(E)$ of being in a state corresponding to the given energy E. $T = 2.4$. Numerically approximated $\sigma_E^2 = 96.51$. We see that we have alot more variance. Note also that the distribution approaches a Gaussian curve.

5.6 $\langle E \rangle$, $\langle |M| \rangle$, C_V, and χ as functions of T

In order to study the behaviour of the Ising model close to the critical temperature, we do a series of calculations for different temperatures T close to this temperature, T_c. The calculations are done for differing values of L. The resulting expectation values as functions of temperature are shown in figures 15, 16, 17, and 18.

In the mean field approximation this quantity goes to zero at the critical temperature, we do not see this, but we see that the energy curve has an inflection point at the critical temperature. This means that its derivative with respect to temperature, C_V, will have a stationary point there, which we can also see. See figures 15 and 17.

When we did the mean field approximation in section 2.2 we produced a plot of the average magnetization versus the temperature. Looking at the corresponding graph from our simulations we can recognize the general shape, but the critical phenomena from the mean field approximation, (infinite slope at T_C and $m = 0$ at higher temperatures), are not the same in the simulation. However we can see that as L increases, the two graphs share atleast some resemblance. Note also that although the curve from the simulation does not reach zero at the critical point, it does, like the energy, have an inflection point there. See figures 16 2.

The susceptibility, χ, has a stationary point at the critical temperature, like the specific heat, but it is not entirely obvious why. χ is the derivative of the magnetization, but not with respect to temperature. It may be that χ somehow must have a stationary point since the magnetization has an inflection point, but we are not sure. See figure 18.

5.7 Solving for T_C

We are solving this equation in order to find $T_C(\infty)$:

$$T_C(L) - T_C(\infty) = aL^{-\frac{1}{\nu}}, \tag{12}$$

where $\nu = 1$.

We use the maximum of the C_V graph as our approximation for $T_C(L)$. Solving equation 12 we get a few different values for a, averaging over all numbers we find $a \approx 0.75$. Using the value of $T_C(80)$ in equation 12 we get:

$$T_C(\infty) \approx 2.266\,.$$

We note that this correponds well to the exact value derived by Lars Onsager,

$$T_C = \frac{2}{\ln(1+\sqrt{2})} \simeq 2.269\,.$$

6 Conclusion

This was an engaging project with a lot of physics, but because of time constraints we feel that we have not had time to really penetrate all aspects of the problem. An interesting aspect of the problem, that we have not looked at, would be to study at plots of the lattice itself (1 is black -1 is white for example). It would also be fun to study the different power laws describing the behaviour of the system near the critical temperature.

We found that the Metropolis algorithm was fairly easy to implement and produce results with, although scaling up the lattice size soon became very heavy computationally. As an example, we tried running $N = 10^8$ Monte Carlo cycles on a 100×100-lattice, and found that it took about 17 hours (!) to complete (using four cores on one of the computers at the lab).

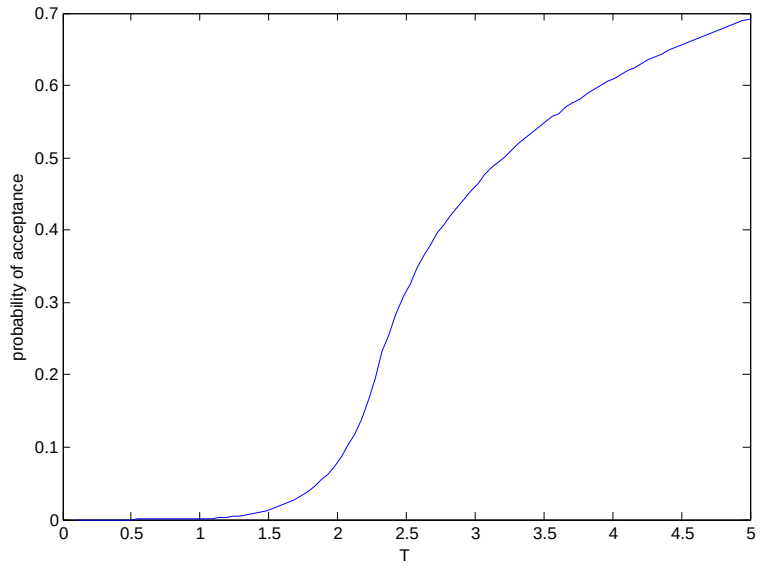

Figure 14: Probability of accepting configurations plotted versus temperature for the 20×20-case. $N = 10^4$, starting in the ground state. For low temperatures, the system is mostly in the ground state, meaning almost all proposed flips will result in a higher energy. However, when the temperature increases, the denominator in the exponent of the Boltzmann factor becomes dominating, making accepting proposed flips very probable.

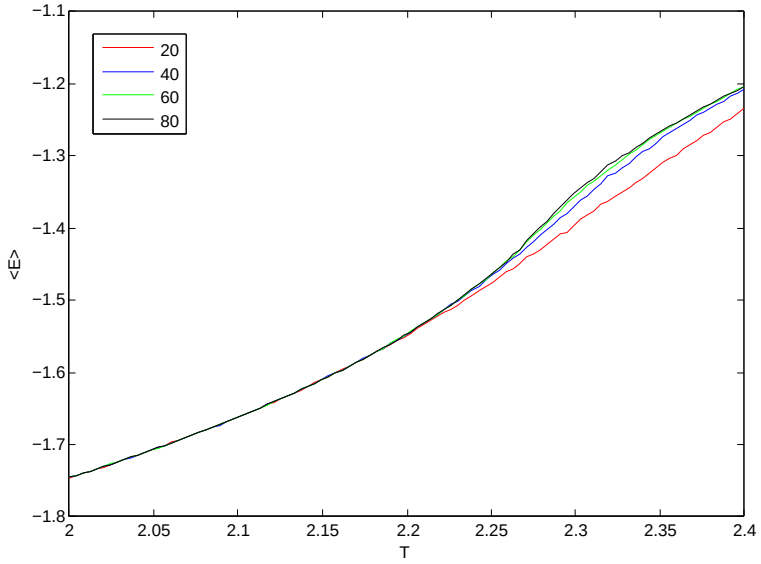

Figure 15: $\langle E \rangle$ as a function of temperature, T, for lattice sizes $n = 20, 40, 60$, and $n = 80$ (shown in red, blue, green, and black, respectively). $N = 10^6$ Monte Carlo cycles used after reaching equilibrium.

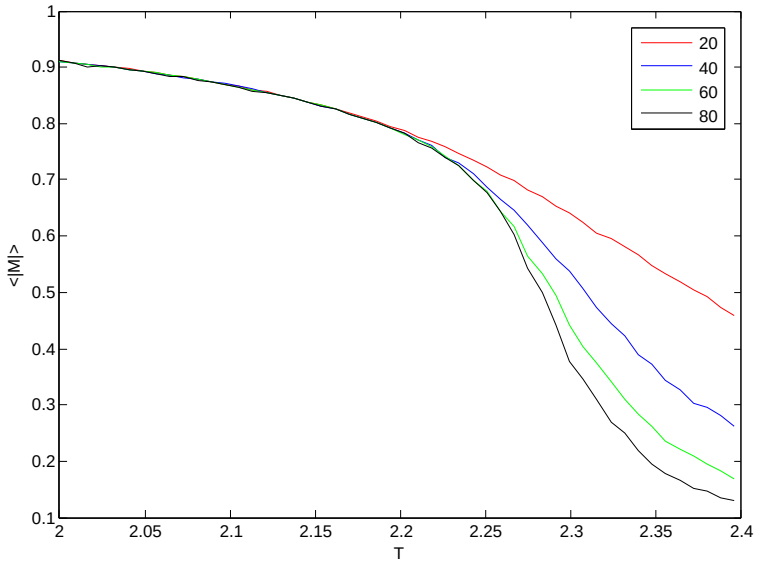

Figure 16: $\langle |M| \rangle$ as a function of temperature, T, for lattice sizes $n = 20, 40, 60$, and $n = 80$ (shown in red, blue, green, and black, respectively). $N = 10^6$ Monte Carlo cycles used after reaching equilibrium.

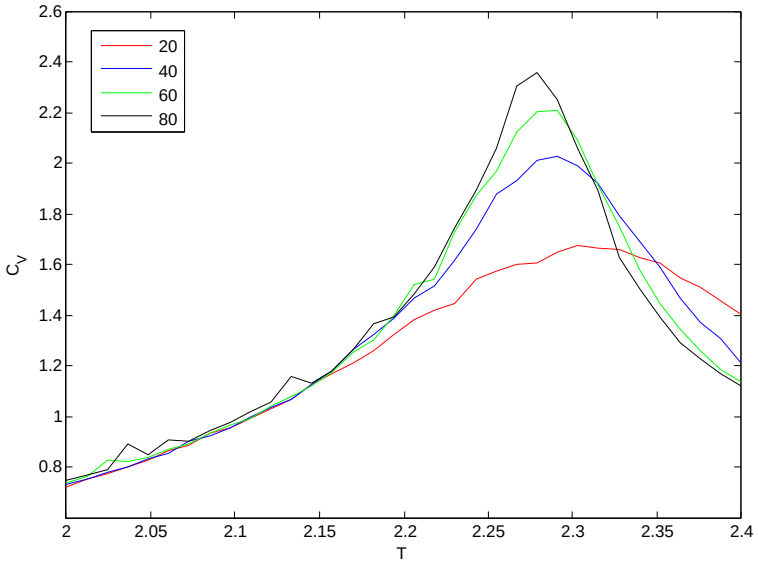

Figure 17: C_V as a function of temperature, T, for lattice sizes $n = 20, 40, 60$, and $n = 80$ (shown in red, blue, green, and black, respectively). $N = 10^6$ Monte Carlo cycles used after reaching equilibrium.

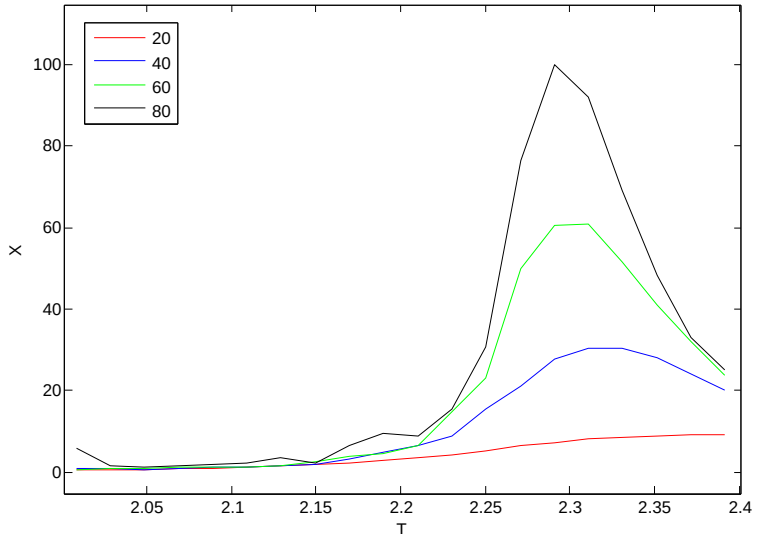

Figure 18: χ as a function of temperature, T, for lattice sizes $n = 20, 40, 60$, and $n = 80$ (shown in red, blue, green, and black, respectively). $N = 10^6$ Monte Carlo cycles used after reaching equilibrium.